Compound Screening Libraries

Accelerating Early Drug Discovery
Drug discovery and development is a time-consuming and high-cost process; including early drug discovery, pre-clinical studies, clinical development, FDA review, and post-market monitoring. Early drug discovery is a key step in drug discovery and development process. Nowadays, early drug discovery involves target identification & validation, screening hits, and optimization of hits, etc. With the development of chemical synthesis and natural products extraction technology, large numbers of small molecule compounds are available for screening. High throughput screening (HTS) technology accelerated the hit discovery process. In recent decades, approaches such as fragment-based drug discovery (FBDD), structure-based drug discovery (SBDD), drug repurposing and repositioning, and virtual screening, have been exploited to reduce the cost and increase the success rate of drug discovery and development.

MCE Compound Library

- HTS compound database, molecular docking and virtual screening service
- 30,000+ bioactive compounds with clear target and function annotation
- 18,000+ fragment compounds with diverse structures
- Customized libraries are also available

**Fragment Library**
- 18,000+ fragment compounds
- Diverse structure
- Useful tool for fragment-based drug discovery (FBDD)

**Bioactive Compound Library**
- 100+ bioactive compound libraries
- 30,000+ bioactive compounds are supplied
- Covering 500+ targets and hot research areas

**Customized Compound Library**
- Specific Compounds
- Plate Map
- Size
- Form (Solid or DMSO Solution) …

High Throughput Screening Library
- 16 million compounds are available
- Diverse structure and Drug-like features
- All compounds are in stock and can be resupplied
Virtual screening is a computational technique that automatically searches large libraries of small molecules in order to identify those structures which most likely to bind to a drug target. It has become an integral part of the early drug discovery process.

MedChemExpress (MCE) provides high quality virtual screening service that enables researchers to efficiently identify scaffolds with promising structure activity relationship (SAR). Our optimized virtual screening protocol can reduce the size of chemical library to be screened experimentally, increase the likelihood to find innovative hits in a faster and less expensive manner, and mitigate the risk of failure in the lead optimization process.

MCE offers versatile HTS compound databases covering 16 million in-stock, reproducible, structurally diverse, drug-like compounds. MCE’s virtual screening service truly realizes ultra-high-throughput compound library + cloud computing platform = unlimited possibilities.

A classic case:
The structure model diagram of Sotorasib binding KARS G12C: The acrylamide double bond of Sotorasib covalently binds to the amino acid residue Cys12 of KARS G12C. The carboxyl group on the benzene ring of Sotorasib acts as a hydrogen bond donor to form a hydrogen bond with residue Glu62, and the hydrogen bond distance is 2.3 Å. In addition, the compound not only forms a π-π stacking interaction with the residue His95, but 2-fluoro-6-hydroxyphenyl can also form a cation-π interaction with the residue Lys88.
MCE Bioactive Screening Libraries

Our ready-to-use MedChemExpress (MCE) compound libraries consist of over 30,000 small molecules with validated biological and pharmacological activities. They are available for high-throughput screening (HTS) and high-content screening (HCS). Bioactive compound libraries are useful tools for drug repurposing and new indication research.

- Safety and effectiveness have been confirmed by literatures, patent reports and clinical researches.
- Focuses on hundreds of targets that are key components in the fields of GPCRs, kinases, cancer, epigenetics and stem cell biology, etc.
- Libraries are updated every week by adding newly published small molecules in the related fields, providing customers with a more comprehensive and innovative choice.
- MCE provides detailed biological and chemical information on every compound together with the LC/MS and NMR reports to ensure high quality.
- MCE offers customized compound libraries based on your specific needs. You can select the compounds’ format (powder/liquid), size and plate map depending on your requirements.

Customize Your Library

According to the signaling pathways, research areas, clinical data and other features of products, compound libraries can be classified into several types, such as FDA-approved drug library, kinase inhibitor library, etc. We can now supply more than 100 types of compound libraries, including drug repurposing libraries, natural products, anti-microbial compounds libraries, cancer related libraries, and cell death related libraries.
Our Advantages

**Complete Product Categories and Quick Updates**

30,000 + bioactive compounds, 16 million screening compounds and 16,000 + fragment compounds can be selected based on your specific needs. New compounds are launched and added to our libraries regularly to ensure their comprehensiveness.

**Perfect Product and Data Management System**

Our compound library preparation is automated and all products can be traced to avoid human error. Each product is supplied with detailed bioactivity information and physicochemical properties.

**Rigorous Classification Criteria**

Based on a large number of literatures and authoritative database analysis, we set accurate classification standards for each library.

**Strict Quality Management System**

Certified by ISO 9001 quality management system, with state-of-the-art R&D and manufacturing facilities, strict quality control and verification system.

**Professional Service**

MCE can provide you with the professional technical support along with the high-quality products at the most competitive price and the shortest delivery time.

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**Customize Library**

You can select:
- Specific Compounds
- Quantities
- Plate Map
- Concentration
- Form (Solid or Solution)
## Bioactive Compound Library Parameters

<table>
<thead>
<tr>
<th>Specifications</th>
<th>96-well Format Sample Storage Tube</th>
<th>96-/384- well plate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concenetration</td>
<td>30 μL, 50 μL, 100 μL or other size lower than 750 μL</td>
<td>96-well plate: 30 μL, 50 μL, 100 μL or other size lower than 100 μL 384-well plate: 30 μL, 50 μL or other size lower than 50 μL</td>
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<tr>
<td>Sealing Way</td>
<td>Screw Cap</td>
<td>Peelable Foil Seal</td>
</tr>
<tr>
<td>Concentration</td>
<td>10 mM solution for products with stable solution state and solubility no less than 10 mM; 2 mM solution for products with solubility between 2 mM and 10 mM; 3 mg/mL solution for products with unconfirmed molecular weight and solubility no less than 3 mg/mL.</td>
<td></td>
</tr>
<tr>
<td>Solvent</td>
<td>DMSO, Water, Ethanol.</td>
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</tr>
<tr>
<td>Recommended Storage Time</td>
<td>-20°C for 1 year; -80°C for 2 years</td>
<td></td>
</tr>
<tr>
<td>Information Shipped with Library</td>
<td>Product information including targets, bioactivity information, research areas, clinical data, etc.; Product layout for each plate; SDF file, contains structure information and requires some specialized software to open (ChemOffice).</td>
<td></td>
</tr>
<tr>
<td>Plate Layout</td>
<td><img src="image" alt="96-well Plate Layout" /></td>
<td><img src="image" alt="384-well Plate Layout" /></td>
</tr>
</tbody>
</table>

Compounds with different concentrations or dissolved in different solutions are put on different plates. If you have any other requirements for the compounds layout, please let us know before you make the order.
Publications Citing Use of MCE Products:

Nature. 2022 May;605(7910):567-574.
Nature. 2022 May;605(7911):747-753.
Nature. 2022 May;605(7909):325-331.
Nature. 2022 Apr;604(7906):541-545.
Nature. 2022 Apr;604(7904):134-140.
Nature. 2022 Mar;603(7899):159-165.
Nature. 2022 Mar;603(7899):138-144.
Science. 2022 Mar 18;375(6586):1254-1261.
Cell. 2022 Jun 9;S0092-8674(22)00651-1.
Cell. 2022 May 11;S0092-8674(22)00526-8.
Cell. 2022 Apr 28;185(9):1521-1538.e18.
Cell. 2021 Sep 2;184(18):4753-4771.e27.
Cell. 2021 Jun 10;184(12):3143-3162.e32.
Cell. 2021 Apr 1;184(7):1693-1705.e17.
MCE Global Partners
<table>
<thead>
<tr>
<th>Page</th>
<th>Section</th>
<th>Libraries</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Bioactive Compound Libraries</td>
<td>HY-L001, HY-L001P Bioactive Compound Library</td>
</tr>
<tr>
<td>11</td>
<td>Drug Repurposing Series</td>
<td>HY-L022, HY-L022P &amp; HY-L022M FDA-Approved Drug Library</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HY-L066 FDA Approved &amp; Pharmacopeial Drug Library</td>
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<td>HY-L033 NMCPA-Approved Drug Library</td>
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<td>HY-L035 &amp; HY-L035P Clinical Compound Library</td>
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<td>HY-L035 &amp; HY-L035P Drug Repurposing Compound Library</td>
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<td>Natural Products Series</td>
<td>HY-L021 &amp; HY-L021P Natural Product Library</td>
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<tr>
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<td>HY-L056 Terpenoids Library</td>
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<td>HY-L071 Alkaloids Library</td>
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<td>HY-L057 Phenols Library</td>
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<td>HY-L021L Natural Product Like Compound Library</td>
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<td></td>
<td>HY-L065 Traditional Chinese Medicine Monomer Library</td>
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<td>HY-L065 Medicine Food Homology Compound Library</td>
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<tr>
<td>21</td>
<td>Cell Death Series</td>
<td>HY-L051 Ferroptosis Compound Library</td>
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<td>HY-L003 Apoptosis Compound Library</td>
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<td>Metabolism Series</td>
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<td>HY-L064 Glutamine Metabolism Compound Library</td>
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<td>HY-L058 Human Endogenous Metabolite Compound Library</td>
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<td>HY-L094 Microbial Metabolite Library</td>
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<td>HY-L078 Gut Microbial Metabolite Library</td>
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<td>HY-L091 Lipid Metabolism Compound Library</td>
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<td>HY-L092 Glucose Metabolism Compound Library</td>
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<td>28</td>
<td>According to Product Features &amp; Structures</td>
<td>HY-L061 Orally Active Compound Library</td>
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<td>HY-L063 Chemical Probe Library</td>
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<td>HY-L076 Drug-Induced Liver Injury (DILI) Compound Library</td>
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<td>HY-L094 Food-Sourced Compound Library</td>
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<td>HY-L093 Food Additive Library</td>
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<td>HY-L093 Peptidomimetic Library</td>
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<td>HY-L036 &amp; HY-L036P Covalent Screening Library</td>
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<td>HY-L041 Macrocyclic Compound Library</td>
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<td>HY-L044 Nucleotide Compound Library</td>
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<td>HY-L032 Fragment Library</td>
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<td>32</td>
<td>According to Signaling Pathway or Protein Family</td>
<td>HY-L037 Antioxidants Compound Library</td>
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<td>HY-L038 Differentiation Inducing Compound Library</td>
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<td>HY-L039 Reprogramming Compound Library</td>
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<td>HY-L050 Ubiquitination Compound Library</td>
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<td>HY-L051 Natural Product Like Compound Library</td>
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<td>HY-L066 Traditional Chinese Medicine Monomer Library</td>
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<td>HY-L065 Medicine Food Homology Compound Library</td>
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</table>
**Cat. No.: HY-L001, HY-L001P**

**Bioactive Compound Library**

(96-/384-well plate)

<table>
<thead>
<tr>
<th>Cat. No.</th>
<th>Product Name</th>
<th>Compound Number</th>
<th>Supply Form</th>
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</thead>
<tbody>
<tr>
<td>HY-L001</td>
<td>Bioactive Compound Library</td>
<td>13,000+</td>
<td>Part A: Solution or Solid</td>
</tr>
<tr>
<td>HY-L001P</td>
<td>Bioactive Compound Library Plus</td>
<td>15,000+</td>
<td>Part A, Part B &amp; Part C Part B: Only solid Part C: Only solid</td>
</tr>
</tbody>
</table>

**Part B-low solubility or less stable solution:** For the compounds with less solution stability and due to the short shelf life of the solution, powder packaging is recommended and can be dissolved at the time of use. For the products with low solubility, MCE also provides them in powder form.

**Part C-novel, rare or exclusive compounds:** The products in Part C are some novel, rare or exclusive compounds, which are of high prices. MCE lists them separately and provides at least 1 mg powder packaging or ≥250 µL solution packaging. You can also choose based on your specific needs.

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**Publications Citing Use of MCE Bioactive Library Compounds**

- Nat Metab. 2021 May;3(5):682-700.

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**Product Features**

- A unique collection of **10,000+** small molecules with validated biological and pharmacological activities.
- Cover more than **500** kinds of targets, involving more than **20** major signaling pathways and several hot research areas.
- Products contain natural products, innovative compounds, approved compounds, and clinical compounds, etc. Used for signaling pathway research, drug discovery and drug repurposing, etc.
- High purity and quality validated by NMR and LC/MS.

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![Clinical phase for bioactive compounds](image1)

![Signaling pathways of bioactive compounds](image2)
Drug repurposing is a new trend in drug development. Compared with new drug development, drug repurposing has the following advantages:

Drug safety has been widely verified at the clinical stage and in the pharmaceutical market, which reduces the risk of drug development failure caused by safety. The drugs have gone through systematic pre-clinical and clinical studies, with comprehensive research and complete data. Thus, they can greatly shorten the research and development cycle. Compared with development of new drugs for the same indication, drug repurposing can greatly save research costs.

Advantage comparison between drug repurposing and development of new drugs.

Getting a drug to market currently takes 12–16 years and between US$1 billion and $2 billion on average, and the costs are going up. But some estimates suggest that repositioning drug costs on average $300 million and takes around 6.5 years. [1]

Product Features

- All compounds have been approved by FDA, EMA, NMPA and other countries. Approved agencies for every drug are available. Nearly 70% of the drugs in this library are FDA-approved.
- Rigorous classification criteria: MCE FDA-Approved Drug Library does not contain veterinary drugs, Inactive Ingredients, food additives or compounds that are included in NDC or DMF but have not been approved for drugs.
- Cover more than 200 common targets and a variety of hot research areas, such as oncology, infection, immunity, cardiovascular disease and nervous system diseases.
- FDA-Approved Drug Library Plus (HY-L022P) further complements FDA-Approved Drug Library (HY-L022) by adding some compounds with low solubility or less solution stability and some novel, rare or exclusive compounds (Part B) to this library. All those supplementary are supplied in powder form.

**Research areas involved in the FDA-approved drug library**

- Cancer
- Infection
- Neurological Disease
- Metabolic Disease
- Cardiovascular Disease
- Endocrinology
- Inflammation/Immunology
- Others

**Signaling pathways involved in the FDA-approved drug library**

- JAK/STAT Signaling
- Cytoskeleton
- MAPK/ERK Pathway
- PI3K/Akt/mTOR
- Inflammation/Immunology
- Cell Cycle/DNA Damage
- Cell Cycle/DNA Damage
- Apoptosis
- Autophagy
- NF-κB
- Epigenetics
- Protein Tyrosine Kinase/RTK
- Others
- GPCR/G Protein
- Neuronal Signaling
- Stere Cell/Wnt
- MAPK/ERK Pathway

**Publications Citing Use of MCE FDA-Approved Library Products**


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**Cat. No.: HY-L022, HY-L022P & HY-L022M**

**FDA-Approved Drug Library**

(96-/384-well plate)

<table>
<thead>
<tr>
<th>Cat. No.</th>
<th>Product Name</th>
<th>Compound Number</th>
<th>Supply Form</th>
<th>Package</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>HY-L022</td>
<td>FDA-Approved Library</td>
<td>2,400+</td>
<td>Part A: Solution or powder</td>
<td>96-well storage tubes; 96-well/384-well microplate</td>
<td>High cost performance</td>
</tr>
<tr>
<td>HY-L022</td>
<td>FDA-Approved Library Plus</td>
<td>2,600+</td>
<td>Part A &amp; Part B Part B: Powder only</td>
<td>96-well storage tubes; 96-well/384-well microplate</td>
<td>A more powerful screening capability</td>
</tr>
<tr>
<td>HY-L022</td>
<td>FDA-Approved Library Min</td>
<td>1,900+</td>
<td>Solution only (10 μL/well)</td>
<td>96-well microplate</td>
<td>Low price, fast delivery</td>
</tr>
</tbody>
</table>

www.MedChemExpress.com

Inhibitors  •  Screening Libraries  •  Proteins
Examples of Targets included in This Library

- 5-Alpha Reductase
- Adrenergic Receptor
- ACE
- Autophagy
- Carbonic Anhydrase
- COX
- DNA/RNA Synthesis
- Estrogen Receptor/ERR
- FGFR
- HCV
- Histone Methyltransferase
- Integrin
- Microtubule/Tubulin
- P2Y Receptor
- Phosphatase
- Progesterone Receptor
- ROCK
- S-HT Receptor
- Akt
- Antibiotic
- Bacterial
- Chloride Channel
- CXCR
- Drug Metabolite
- Factor Xa
- Fungal
- HDAC
- HIV
- Interleukin Related
- MMP
- Parasite
- Phosphodiesterase (PDE)
- Proton Pump
- SGLT
- AChE
- Aldose Reductase
- Antifolate
- Btk
- Cholecystokinin Receptor
- Cytochrome P450
- EGFR
- Farnesyl Transferase
- Gap Junction Protein
- HIF/HIF Prolyl-Hydroxylase
- iGluR
- LPL Receptor
- nAChR
- PARP
- PKC
- Reactive Oxygen Species
- Topoisomerase
- 5-HT Receptor
- Akt
- Antibiotic
- Bacterial
- Chloride Channel
- CXCR
- Drug Metabolite
- Factor Xa
- Fungal
- HDAC
- HIV
- Interleukin Related
- MMP
- Parasite
- Phosphodiesterase (PDE)
- Proton Pump
- SGLT
- AChE
- Aldose Reductase
- Antifolate
- Btk
- Cholecystokinin Receptor
- Cytochrome P450
- EGFR
- Farnesyl Transferase
- Gap Junction Protein
- HIF/HIF Prolyl-Hydroxylase
- iGluR
- LPL Receptor
- nAChR
- PARP
- PKC
- Reactive Oxygen Species
- Topoisomerase
- Adenosine Receptor
- Angiotensin Receptor
- Apoptosis
- Calcium Channel
- c-Kit
- DHODH
- Endogenous Metabolite
- Ferroptosis
- GSK-3
- Histamine Receptor
- Influenza Virus
- mACHR
- NKCC
- PDGFR
- Potassium Channel
- RET
- VEGFR

Publications Citing Use of MCE FDA Approved & Pharmacopeial Library Products

NMPA-Approved Drug Library
(96-/384-well plate)

Product Features
- A unique collection of 1,200+ NMPA-approved compounds that could be used for HTS and HCS.
- All the compounds have undergone extensive preclinical and clinical trials, showing good bioactivity, safety and bioavailability.
- A useful tool for drug repurposing which could dramatically accelerate drug development.
- More detailed compound information with structure, IC\textsubscript{50}, and brief introduction.
- High purity and quality validated by NMR and LC/MS.

Clinical Compound Library
(96-/384-well plate)

Product Features
- All compounds were reported in the authoritative clinical database. Clinical information for each compound is available.
- Compounds in this library include clinical compounds and drugs withdrawn from the market (Phase IV).
- Cover 260+ commonly used targets and a variety of hot research areas, such as cancer, immunity, infection, cardiovascular, etc.
- HY-L026P, with a more powerful screening capability, further supplements HY-L026 by adding some compounds with low stability or low solubility and some novel, rare or exclusive compounds (Part B). Supplementary compounds are provided in powder form.

<table>
<thead>
<tr>
<th>Cat. No.</th>
<th>Product Name</th>
<th>Compound Number</th>
<th>Supply Form</th>
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<tbody>
<tr>
<td>HY-L026</td>
<td>Clinical Compound Library</td>
<td>1,700+</td>
<td>Part A: Solution or powder</td>
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<tr>
<td>HY-L026P</td>
<td>Clinical Compound Library Plus</td>
<td>1,900+</td>
<td>Part A &amp; Part B Part B: Powder only</td>
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</tbody>
</table>
Drug Repurposing Compound Library
(96-/384-well plate)

Cat. No.: HY-L035 & HY-L035P

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<tbody>
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<td>HY-L035</td>
<td>Drug Repurposing Compound Library</td>
<td>3,800+</td>
<td>Part A: Solution or powder</td>
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<tr>
<td>HY-L035P</td>
<td>Drug Repurposing Compound Library Plus</td>
<td>4,100+</td>
<td>Part A &amp; Part B Part B: Powder only</td>
</tr>
</tbody>
</table>

Product Features

- Compounds include approved drugs and clinical drugs passing phase I.
- Compounds in this library have identified bioactivities, good pharmacokinetic characteristics and safety, which are suitable for drug repurposing.
- Detailed bioactivity information including target, clinical data, etc. is available.
- Cover more than 300 kinds of commonly used targets, involving a variety of hot research areas.
- HY-L035P, with a more powerful screening capability, further supplements HY-L035 by adding some compounds with low stability or low solubility and some novel, rare or exclusive compounds (Part B). Supplementary compounds are provided in powder form.

Examples of Targets in these Libraries

- 5-Alpha Reductase
- Adenosine Receptor
- AMPK
- ACE
- Btk
- CGRP Receptor
- COMT
- DNA/RNA Synthesis
- Endogenous Metabolite
- Factor Xa
- HCV
- mAChR
- Opioid Receptor
- Serotonin Transporter
- 5-HT Receptor
- Akt
- Amyloid-β
- Aromatase
- Calcium Channel
- Chloride Channel
- COX
- Dopamine Receptor
- Endothelin Receptor
- iGluR
- Microtubule/Tubulin
- Phosphodiesterase (PDE)
- SGLT
- AChE
- Aldose Reductase
- Androgen Receptor
- Bcl-2 Family
- CaSR
- Cholecystokinin Receptor
- CRISPR/Cas9
- EGFR
- Epoxide Hydrolase
- GABA Receptor
- JAK
- Monoamine Oxidase
- Potassium Channel
- Sodium Channel
- ADC Cytotoxin
- ALK
- Angiotensin Receptor
- Bradykinin Receptor
- CDK
- c-Kit
- Cytochrome P450
- Elastase
- Estrogen Receptor/ERR
- Glucocorticoid Receptor
- LPL Receptor
- Neurokinin Receptor
- Progesterone Receptor
- Thyroid Hormone Receptor
The structural diversity of natural products and their easy binding with biomacromolecules determine their incomparable advantages in the process of life regulation and endue natural products with an irreplaceable important position in the research and development of new drugs. Natural products and their molecular frameworks are the main sources of new drugs, in fact, about two-thirds of all drugs approved between 1981 and 2019 are, at different extents, related to natural products [1].

MCE can provide natural products and natural product analogues from a variety of sources, including plants, animals, and microorganisms. The compounds in the library contain Saccharides & Glycosides, Phenylpropanoids, Quinones, Flavonoids, Terpenoids and Glycosides, Steroids, Alkaloids, Phenols, Acids and Aldehydes.

MCE natural products have clear source information and structure classification for data analysis. Natural products and analogues available from MCE are as follows:

- HY-L021 & HY-L021P ........................................... 17
  Natural Product Library
- HY-L056 .......................................................... 18
  Terpenoids Product Library
- HY-L071 .......................................................... 18
  Alkaloids Product Library
- HY-L068 .......................................................... 18
  Flavonoids Product Library
- HY-L057 .......................................................... 18
  Phenols Library
- HY-L021L .......................................................... 19
  Natural Product Like Compound Library
- HY-L065 .......................................................... 20
  Traditional Chinese Medicine Monomer Library
- HY-L055 .......................................................... 20
  Medicine Food Homology Compound Library

Natural Product Library
(96-/384-well plate)

Product Features

- All natural products have clear sources and structure classifications.
- Structurally diverse, including Saccharides and Glycosides, Phenylpropanoids, Quinones, Flavonoids, Terpenoids and Glycosides, Steroids, Alkaloid, Phenols, Acids and Aldehydes, etc.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- Bioactivity diversity, covering 200+ common targets, 20+ hot signaling pathways and a variety of research areas.
- HY-L021P, with a more powerful screening capability, further supplements HY-L021 by adding some compounds with low solution stability or low solubility and some novel, rare or exclusive compounds (Part B). Supplementary compounds are provided in powder form.

<table>
<thead>
<tr>
<th>Cat. No.</th>
<th>Product Name</th>
<th>Compound Number</th>
<th>Supply Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>HY-L021</td>
<td>Natural Product Library</td>
<td>3,200+</td>
<td>Part A: Solution or powder</td>
</tr>
<tr>
<td>HY-L021P</td>
<td>Natural Product Library Plus</td>
<td>3,600+</td>
<td>Part A &amp; Part B</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Part B: Powder only</td>
</tr>
</tbody>
</table>

Source of products in MCE Natural Product Library

Different structure types in MCE Natural Product Library

Publications Citing Use of MCE Natural Product Library Compounds

- Cancer Lett. 2020 Jul 1;1,481:15-23.
- Theranostics. 2021 Apr 19;11(13):6355-6369.
Terpenoids, Alkaloids, Flavonoids and Phenols Product Libraries (96-/384-well plate)

Product Features

- Structurally diverse, bioactive, and cell permeable.
- Bioactivity and safety have been confirmed by clinical and/or preclinical trials. Some compounds have been approved by FDA.
- More detailed compound information with structure, target, and brief introduction.
- High purity and quality validated by NMR and LC/MS.

<table>
<thead>
<tr>
<th>Product Name</th>
<th>Induction</th>
<th>Product Features</th>
<th>Representative Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>HY-L056</td>
<td>Terpenoids display a wide array of important pharmacological properties in the fight against cancer, malaria, inflammation, and a variety of infectious diseases.</td>
<td>A unique collection of <strong>400+</strong> natural terpenoid compounds, such as monoterpenes, sesquiterpenes, diterpenes, ester terpenes and triterpenes, etc.</td>
<td><img src="image1" alt="Terpenoid Structure" /></td>
</tr>
<tr>
<td>HY-L071</td>
<td>Alkaloids are a large and complex group of cyclic compounds that contain N. Important alkaloids include morphine, strychnine, atropine, colchicine, ephedrine, quinine, and nicotine. They show anti-inflammatory, anticancer, analgesics, local anesthetic and neuropharmacological activities, etc.</td>
<td>A unique collection of <strong>500+</strong> natural alkaloids, such as indoles, quinolines, isoquinolines, pyrrolidines, pyridines, pyrrolizidines, tropanes, and terpenoids and steroids.</td>
<td><img src="image2" alt="Alkaloid Structure" /></td>
</tr>
<tr>
<td>HY-L068</td>
<td>Flavonoids have anti-oxidative, anti-mutagenic, anti-inflammatory, and anti-carcinogenic properties coupled with capacity to modulate key cellular enzyme function. They have been widely used in a variety of nutrition, medicine and cosmetics.</td>
<td>A unique collection of <strong>350+</strong> natural flavonoid compounds, such as flavones, flavonols, flavanones, flavanonols, flavanols, etc.</td>
<td><img src="image3" alt="Flavonoid Structure" /></td>
</tr>
<tr>
<td>HY-L057</td>
<td>Phenolic compounds are a diverse group of naturally occurring compounds with multiple activities, such as antioxidant and antimicrobial properties.</td>
<td>A unique collection of <strong>800+</strong> natural phenol compounds with a variety of biological activities.</td>
<td><img src="image4" alt="Phenol Structure" /></td>
</tr>
</tbody>
</table>
Natural products (NPs) and their molecular frameworks are the main sources of new drugs and play highly significant roles in the drug discovery and development process. Based on the source and structure analysis of 1,562 drugs approved by the FDA from 1981 to 2014, it was found that 21% of the drugs were natural product derivatives, and 61% of the drugs contained natural product pharmacophore groups. From this point, it concludes that natural product analogues and derivatives have the same screening value as natural products in the development of new drugs.

MCE provides a unique collection of 200+ natural product-like compounds that are structurally like Steroids, Tannins, Flavonoids, Isoquinolines, etc. This library is an important source of lead compounds for HTS and HCS.

**Product Features**

- All products are natural product analogues or derivatives and can be used in the development of new drugs.
- Structurally diverse, bioactive, and cell permeable.
- Detailed bioactivity information, including target, research areas and clinical information.
- High purity and quality validated by NMR and LC/MS.

**Examples of Products in the Library**

<table>
<thead>
<tr>
<th>Quinones</th>
<th>Flavonoids</th>
<th>Cephalosporins</th>
</tr>
</thead>
<tbody>
<tr>
<td>HY-13502</td>
<td>HY-10005</td>
<td>HY-B1117</td>
</tr>
<tr>
<td>Mitoxantrone</td>
<td>Flavopiridol</td>
<td>Cefoxitin sodium</td>
</tr>
<tr>
<td>HY-15842</td>
<td>HY-12028</td>
<td>HY-B1156</td>
</tr>
<tr>
<td>SF1670</td>
<td>PD98059</td>
<td>Cephradine</td>
</tr>
<tr>
<td>HY-111441</td>
<td>HY-12422</td>
<td>HY-B1381</td>
</tr>
<tr>
<td>1,4-Chrysenequinone</td>
<td>Voruciclib</td>
<td>Cefixime</td>
</tr>
</tbody>
</table>
Traditional Chinese Medicine (TCM) has been used for centuries in China, where herbs are considered fundamental therapy for many acute and chronic conditions. Many studies indicated TCM exerted an overall regulatory effect via multi-component and multi-target network. Traditional Chinese medicine monomers are active compounds of Chinese Herbal Medicines. They possess medicinal properties such as anti-cancer, anti-bacterial effects may be an important source of new drugs. For example, Artemisinin, used in multidrug resistant malaria, was first isolated from the Chinese herb Artemisia annua L.

MCE designs a unique collection of 1,700+ compounds that all come from Chinese Herbal Medicines. MCE Traditional Chinese Medicine Monomer Library is a useful tool for discovering new drugs from TCM.

Product Features
- Structurally diverse, containing Saccharides & Glycosides, Terpenoids & Glycosides, Alkaloid, Phenols, Acids and Aldehydes, etc.
- Sources diverse, including ginseng, coptis, notoginseng, angelica and other 500+ Chinese herbal medicines.
- Clear source of traditional Chinese medicine and detailed bioactivity information is available.
- Bioactivity diverse, covering several hot research areas such as immune inflammation, cancer, anti-infection, cardiovascular disease, etc.

Medicine Food Homology Compound Library
(96-/384-well plate)

Food as medicines have many benefits because of their safety. In order to ensure the safe use of functional food, National Health Commission of the People's Republic of China made specific provisions on Medicine Food Homology (MFH) items. More than 100 kinds of widely used MFH materials have been released.

Based on MFH items released by National Health Commission, PRC, MCE carefully designs a unique collection of 600+ Medicine Food Homology Compounds with high safety.

Product Features
- All compounds are from Medicine Food Homology materials, which have high medicinal value and safety, and can be used for HTS and HCS.
- Sources diverse, those compounds are from more than 100 kinds of Medicine Food Homology materials.
- Detailed bioactivity information, including target, research areas, clinical information.
- High purity and quality validated by NMR and LC/MS.
Programmed cell death (PCD), referring to apoptosis, autophagy and programmed necrosis, is a tightly regulated cellular process that is central to the development, homeostasis and integrity of multicellular organisms. The dysregulation of programmed cell death is closely related to the occurrence and development of many human diseases such as cancer, immune diseases, neurodegenerative diseases and cardiovascular diseases.

Distinctive forms of programmed cell death and their morphological characteristics[1][2].

### MORPHOLOGICAL FEATURES

<table>
<thead>
<tr>
<th>Library</th>
<th>Cell Membrane</th>
<th>Cytoplasm</th>
<th>Nucleus</th>
<th>Biochemical Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferroptosis Library (HY-L051)</td>
<td>Cell rounding</td>
<td>Smaller mitochondria; reduced mitochondrial membrane densities; increased rupture of mitochondrial membrane</td>
<td>Normal</td>
<td>Iron metabolism and ROS production</td>
</tr>
<tr>
<td>Apoptosis Library (HY-L003)</td>
<td>Cell rounding, membrane blebbing</td>
<td>Apoptotic body formation</td>
<td>Normal</td>
<td>Caspase activation; DNA fragment; ΔΨm dissipation</td>
</tr>
<tr>
<td>Autophagy Library (HY-L029)</td>
<td>Normal</td>
<td>Smaller Nucleus; chromatin condensation; DNA damage</td>
<td>Normal</td>
<td>LC3-I to LC3-II conversion; p62 degradation</td>
</tr>
<tr>
<td>Pyroptosis Library (HY-L059)</td>
<td>Cell swelling; rupture of plasma membrane; bubbling;</td>
<td>Release of inflammatory cellular contents</td>
<td>Moderate chromatin condensation; DNA damage</td>
<td>Inflammatory Caspase activation (CASP1, CASP3, and GSDMD)</td>
</tr>
</tbody>
</table>

### BIOCHEMICAL FEATURES

<table>
<thead>
<tr>
<th>Library</th>
<th>Major Regulators</th>
<th>Library Description</th>
<th>Main Targets in Library</th>
<th>Library Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferroptosis Library (HY-L051)</td>
<td>Positive: VDAC2/3, Ras, NOX, TFR1, p53, CARS</td>
<td>600+ ferroptosis signaling pathway related compounds with ferroptosis-inducing or -inhibitory activity.</td>
<td>GPX4, Lipoxynase, HMG-CoA Reductase (HMGCR), Reactive Oxygen Species, Glutamylcysteine Synthetase, Iron Chelator, etc.</td>
<td>Bioactivity and safety have been confirmed in clinical trials and/or preclinical research for HTS and HCS, and some products have been approved by FDA for marketing.</td>
</tr>
<tr>
<td>Apoptosis Library (HY-L003)</td>
<td>Positive: p53, Bax, Other Pro-Apoptotic Bcl-2 Family Proteins</td>
<td>1,500+ apoptosis-related compounds mainly focusing on the key targets in the apoptosis pathway.</td>
<td>Bcl-2 Family, c-Myc, Caspase, FKBP, TNF Receptor, RIP Kinase, etc.</td>
<td>More detailed compound information with structure, IC_{50}, and brief introduction.</td>
</tr>
<tr>
<td>Autophagy Library (HY-L029)</td>
<td>Positive: ATG5, ATG7, Beclin 1</td>
<td>1,100+ autophagy-related compounds for the research of autophagy-related regulation and diseases</td>
<td>FKBP, LRRK2, ULK, etc.</td>
<td>High purity and quality validated by NMR and LC/MS.</td>
</tr>
<tr>
<td>Pyroptosis Library (HY-L059)</td>
<td>Positive: Caspase-1, Caspase-4, Caspase-5, Gasdermin D, NLRP3</td>
<td>800+ pyroptosis-related compounds focusing on the key targets in the pyroptosis pathway.</td>
<td>Caspase-1, Caspase-4, Caspase-11, Caspase-3, Gasdermin D, NOD-Like Receptor (NLR), etc.</td>
<td></td>
</tr>
</tbody>
</table>
Metabolism Series

Metabolism is the set of life-sustaining chemical reactions in organisms. Metabolic pathways are enzyme-mediated biochemical reactions that lead to biosynthesis (anabolism) or breakdown (catabolism) of natural product molecules within a cell or tissue. The main metabolism in the body includes glucose metabolism, lipid metabolism and protein metabolism. Imbalances in metabolic activities have been found to be critical in a number of pathologies, such as diabetes, cardiovascular diseases and metabolic syndrome.

Metabolites are the products and intermediates of cellular metabolism which are usually small molecules. In the process of new drug discovery, metabolites have become an important source of lead compounds because of their safety and the diversity of biological activities. Microbial metabolites play important roles in the development of antibiotic products and non-antibiotic active compounds because of their species diversity and structural novelty.

- HY-L012 Metabolism/Protease Compound Library 24
- HY-L064 Glutamine Metabolism Compound Library 24
- HY-L058 Glycolysis Compound Library 25
- HY-L030 Human Endogenous Metabolite Compound Library 25
- HY-L084 Microbial Metabolite Library 26
- HY-L078 Gut Microbial Metabolite Library 26
- HY-L091 Lipid Metabolism Compound Library 27
- HY-L092 Glucose Metabolism Compound Library 27

Cat. No.: HY-L012

Metabolism/Protease Compound Library
(96-/384-well plate)

Functioned as catalysts, enzymes are crucial to metabolism - they allow a reaction to proceed more rapidly - and they also allow the regulation of the rate of a metabolic reaction. Proteases control a great variety of physiological processes that are critical for life, including the immune response, cell cycle, cell death, wound healing, food digestion, and protein and organelle recycling. Imbalances in metabolic activities have been found to be critical in a number of pathologies, such as cardiovascular diseases, inflammation, cancer, and neurodegenerative diseases. Metabolites are the products and intermediates of cellular metabolism which are usually small molecules. In the process of new drug discovery, metabolites have become important sources of lead compounds because of their safety and diversity of biological activities.

Product Features

- 3,000+ compounds targeting metabolic pathways, such as Carbohydrate metabolism, Lipid metabolism, Amino acid metabolism, etc. A useful tool for HTS and HCS.
- Covers full range of targets, such as PDE, Cytochrome P450, HMG-CoA Reductase, DPP4, Proteasome, HCV Protease, IDO, Cathepsin, MMP, etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L064

Glutamine Metabolism Compound Library
(96-/384-well plate)

Glutamine is an important metabolic fuel that helps rapidly proliferating cells meet the increased demand for ATP, biosynthetic precursors, and reducing agents. Mounting evidences indicate that altered glutamine metabolism in cancer cells has critical roles in supporting macromolecule biosynthesis, regulating signaling pathways, and maintaining redox homeostasis, all of which contribute to cancer cell proliferation and survival. Thus, intervention in glutamine metabolic processes could provide novel approaches to improve cancer treatment.

Product Features

- 600+ glutamine metabolism-related small molecules for HTS and HCS.
- Covers the main targets in glutamine metabolism, such as glucose transporter, glutamate dehydrogenase, glutaminase, c-Myc, etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.
Product Features

- **500+** glycolysis-related small molecules for HTS and HCS.
- Covers the main targets, such as hexokinase, glucokinase, enolase, pyruvate kinase, PDHK, etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L030

**Human Endogenous Metabolite Compound Library**

(96-/384-well plate)

The composition of endogenous metabolite compounds is affected by the upstream influence of the proteome and genome as well as environmental factors, lifestyle factors, medication, and underlying disease. Therefore, metabolites have been described as proximal reporters of disease because their abundances in biological specimens are often directly related to pathogenic mechanisms. In more recent years, metabolomics approach has been adopted or suggested to be used in various research areas including drug discovery, neurosciences, agriculture, food and nutrition, and environmental sciences.

Product Features

- **1,000+** human endogenous metabolites for HTS and HCS.
- All compounds are human endogenous metabolites with better bioavailability.
- A useful tool for metabolomics and metabolism-related drug discovery.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.
Metabolites have become important sources of lead compounds in the development of new drugs due to their safety and diversity of biological activities. Microbial metabolites, in particular, play key roles in the development of antibiotic products and non-antibiotic active compounds due to their species diversity and structural novelty.

**Product Features**

- **600+** microbial metabolites that are important sources of lead compounds and can be used for HTS and HCS.
- A useful tool for metabolomics and metabolism-related drug discovery.
- Structurally diverse, bioactive, and cell permeable.
- High purity and quality validated by NMR and LC/MS.

Accumulating evidence has revealed that intestinal microbiota plays an important role in human health and disease, including cardiovascular diseases, inflammatory bowel disease, diabetes, obesity, cancer, depression. Changes in the composition of gut microbiota associated with disease, called as dysbiosis, have been linked to pathologies. Indeed, the gut microbiome functions like the endocrine organ, generating bioactive metabolites which play important roles in human metabolism, health, and disease. Gut microbiome has become a novel therapeutic target for many diseases. Analysis and identification of gut microbial metabolites will contribute to the development of therapeutic methods.

**Product Features**

- **150+** gut microbial metabolites that can be used for HTS and HCS.
- All the compounds have good bioavailability.
- A useful tool for gut microbiome research and gut microbiome-related drug discovery.
- High purity and quality validated by NMR and LC/MS.
Lipids are a fundamental class of organic molecules implicated in a wide range of biological processes, and based on this can be broadly classified into five categories: fatty acids, triacylglycerols (TAGs), phospholipids, sterol lipids and sphingolipids. Lipids play a crucial role in different metabolic pathways and cellular functions. Lipid metabolism is an important physiological process that is related to nutrient adjustment, hormone regulation, and homeostasis. Lipid metabolism dysregulation is associated with many diseases such as obesity, liver disease, aging, etc.

Product Features

- **300+** lipid metabolism-related compounds that can be used for both HTS and HCS.
- Covers key targets of lipid metabolism pathways, such as acetyl-CoA Carboxylase, Fatty Acid Synthase (FASN), Lipoxygenase, and HMG-CoA Reductase (HMGCR), etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Glucose homeostasis is tightly regulated to meet the energy requirements of the vital organs and maintain an individual’s health. Glucose metabolism includes glycolysis, tricarboxylic acid cycle, pentose phosphate pathway, oxidative phosphorylation and other metabolic pathways. Glucose is the major carbon source that provides the main energy for life. Glucose metabolism dysregulation is also implicated in many diseases such as diabetes, heart disease, neurodegenerative diseases and even cancers.

Product Features

- **600+** glycometabolism-related compounds that can be used for both HTS and HCS.
- Covers the key targets in glucose metabolism pathways, such as Isocitrate Dehydrogenase (IDH), Lactate Dehydrogenase, NADPH Oxidase, Glutathione Peroxidase, etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.
Different physico-chemical properties of the products determine their characteristics and ultimately their applications in different research areas. For example, some compounds with low MW, fewer formal charges (particularly, negative charges) and lower polar surface area tend to be more CNS-penetrant. CNS-penetrant compounds are important tools for the study of neurological disorders, but they also have neurotoxicity\cite{1}. Chemical probe, with high potency, selectivity and cell-permeability, play important roles in both fundamental and applied biological research. By analyzing the different properties of small molecule compounds, MCE can provide a variety of compound libraries with different properties, which you can choose according to your needs.

Different product structures determine different functions. For example, compounds with covalent reactive groups can bind irreversibly to target through covalent bonds which can lead to the development of highly selective inhibitors and overcome drug resistance\cite{1}. Nucleoside and nucleotide analogues can mimic their physiological counterparts and subsequently be incorporated into DNA and RNA to inhibit cellular division and viral replication. Nucleoside and nucleotide analogues can be used to inhibit cancer cell growth, viral replication as well as other indications.

- HY-L028 .................................................. 29
  CNS-Penetrant Compound Library

- HY-L023 .................................................. 29
  Toxins for Antibody-Drug Conjugate Research Library

- HY-L061 .................................................. 29
  Orally Active Compound Library

- HY-L063 .................................................. 29
  Chemical Probe Library

- HY-L076 .................................................. 29
  Drug-Induced Liver Injury (DILI) Compound Library

- HY-L094 .................................................. 29
  Food-Sourced Compound Library

- HY-L093 .................................................. 29
  Food Additive Library

- HY-L033 .................................................. 29
  Peptidomimetic Library

- HY-L036 & HY-L036P .................................. 30
  Covalent Screening Library (Plus)

- HY-L041 .................................................. 30
  Macroyclic Compound Library

- HY-L042 .................................................. 30
  Glycoside Compound Library

- HY-L043 .................................................. 30
  Lipid Compound Library

- HY-L044 .................................................. 30
  Nucleotide Compound Library

- HY-L032 .................................................. 31
  Fragment Library

<table>
<thead>
<tr>
<th>Product Name</th>
<th>Compound Number</th>
<th>Product Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>HY-L028 CNS-Penetrant Compound Library</td>
<td>600+</td>
<td>• A unique collection of bioactive CNS-penetrant compounds.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• A useful tool for the discovery of drugs used for brain diseases, such as brain tumors, mental disorders, and neurodegenerative diseases.</td>
</tr>
<tr>
<td>HY-L023 Toxins for Antibody-Drug Conjugate</td>
<td>40+</td>
<td>• Structurally diverse, including Auristatin derivatives, Maytansinoids, Calicheamicin, Duocarmycin, Pyrrolobenzodiazepines (PBDS).</td>
</tr>
<tr>
<td>Research Library</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HY-L061 Orally Active Compound Library</td>
<td>2,500+</td>
<td>• A unique collection of compounds for discovering new drugs with oral bioavailability.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• All compounds with confirmed oral activity.</td>
</tr>
<tr>
<td>HY-L063 Chemical Probe Library</td>
<td>300+</td>
<td>• A unique collection of chemical probes with high potency, selectivity and cell-permeability.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• A useful tool for fundamental biological research and drug discovery.</td>
</tr>
<tr>
<td>HY-L076 Drug-Induced Liver Injury (DILI)</td>
<td>1,000+</td>
<td>• A unique collection of hepatotoxic compounds.</td>
</tr>
<tr>
<td>Compound Library</td>
<td></td>
<td>• Including antibiotics, anti-cancer agents, anti-inflammatory agents.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Including several different toxicities: steatosis, mitochondrial toxicity, cholestasis, drug allergy (hypersensitivity).</td>
</tr>
<tr>
<td>HY-L094 Food-Sourced Compound Library</td>
<td>1,600+</td>
<td>• All the compounds can be derived from food, which have certain safety.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• All products are provided with detailed food sources.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Structurally diverse, bioactive, and cell permeable.</td>
</tr>
<tr>
<td>HY-L093 Food Additive Library</td>
<td>400+</td>
<td>• All compounds are approved food additives. An important source of lead compounds.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Structurally diverse, bioactive, and cell permeable.</td>
</tr>
<tr>
<td>HY-L033 Peptidomimetic Library</td>
<td>400+</td>
<td>• A unique collection of compounds that act as substitutes for peptides in their interaction with receptors for drug discovery.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Peptoid, α-helix mimetics, β-turn/sheets mimetics and compounds target protein-protein interactions are included.</td>
</tr>
<tr>
<td>Product Name</td>
<td>Compound Number</td>
<td>Product Features</td>
</tr>
<tr>
<td>------------------------------------</td>
<td>-----------------</td>
<td>-------------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>HY-L036 Covalent Screening Library</td>
<td>1,500+</td>
<td>• A unique collection of compounds including molecules identified as covalent inhibitors and other bioactive molecules having common covalent warheads.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Structurally diverse, a variety of covalent warheads, such as acrylamide, alkyl halides, epoxides, azacyclic amines, disulfide, etc.</td>
</tr>
<tr>
<td>HY-L036P Covalent Screening Library Plus</td>
<td>3,000+</td>
<td>• HY-L036P possesses a more powerful screening capability, a complement to HY-L036 by adding some fragment compounds with covalent warheads.</td>
</tr>
<tr>
<td>HY-L041 Macrocyclic Compound Library</td>
<td>200+</td>
<td>• A useful tool for the discovery of &quot;undruggable&quot; targets such as protein-protein interactions (PPIs) inhibitors.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Cyclopeptides, crown ethers, calixarene and so on are included.</td>
</tr>
<tr>
<td>HY-L042 Glycoside Compound Library</td>
<td>300+</td>
<td>• O-glycosides, Ester glycosides, thioglycosides, N-glycoside, sugar-like compounds are included.</td>
</tr>
<tr>
<td>HY-L043 Lipid Compound Library</td>
<td>400+</td>
<td>• A unique collection of lipid and lipid derivative related compounds.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Structurally diverse, triglycerides, phospholipids, sphingolipids, steroids and their structural analogues or derivatives are included.</td>
</tr>
<tr>
<td>HY-L044 Nucleotide Compound Library</td>
<td>300+</td>
<td>• A unique collection of nucleotide/nucleoside and nucleotide/nucleoside analogue compounds.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• A useful tool for discovering anti-cancer and antiviral drugs.</td>
</tr>
</tbody>
</table>

**Publications Citing Use of MCE Products in These Libraries**

- **Autophagy.** 2021 Jun;17(6):1426-1447.
- **Cell Death Dis.** 2021 Mar 3;12(3):229.
- **Cancer Lett.** 2020 Jul 1;481:15-23.
- **Cancer Res.** 2021 Jun 1;81(11):3105-3120.
- **Cancer Lett.** 2021 Mar 16;S0304-3835(21)00117-8.
- **Cell Death Dis.** 2020 Sep 15;11(9):754.

**Customize Library**

- Specific Compounds
- Quantities
- Plate Map
- Concentration
- Form (Solid or Solution)
Fragment-based drug discovery (FBDD) is well suited for discovering both drug leads and chemical probes of protein function. It can cover broad areas of chemical space and allows the use of creative chemistry. Fragment-based drug discovery is well-established in industry and has resulted in a variety of drugs entering clinical trials, with two, vemurafenib and venetoclax, already approved. FBDD also has key attractions for academia. Notably, it is able to engage difficult or novel targets for which no chemical matter may be found in existing HTS collections.

Product Features

- **16,000+** fragment compounds for fragment-based drug discovery (FBDD).
- All compounds follow the Rule of “Three”, in which molecular weight ≤300 Da, the number of hydrogen bond donors (H-donors) ≤3, the number of hydrogen bond acceptors (H-acceptors) is ≤3 and cLogP is ≤3.
- Diversified structures, covering a broader chemical space.
- The solubility of most products in DMSO can reach more than **200 mM**. Higher concentration is also available.
- High purity and quality validated by NMR and LC/MS.

### Parameters

- **Molecular weight**
  - 100-150
  - 150-200
  - 200-250
  - 250-300

- **clogP**
  - <3
  - 3-2
  - 2-1
  - 1-0
  - 0-1
  - 1-2
  - 2-3

- **H-donor**
  - 0
  - 1
  - 2
  - 3

- **H-acceptor**
  - 0
  - 1
  - 2
  - 3
According to Signaling Pathway or Protein Family

Signal transduction or cell signaling concerns the mechanisms by which biological information is transferred between cells or inside the cell. The responses to the extracellular signal are generated by diverse signal transduction mechanisms that frequently involve small intracellular molecules (second messengers) that transmit signals from activated receptors to the cell interior, resulting in changes in the expression of genes and the activity of enzymes. These intercellular and intracellular signaling pathways are essential to the growth, development, metabolism, and the behavior of the organism[1].

Cell signaling pathways are involved in the pathophysiology of many diseases. The mutations, molecular damage or functional change of the proteins in the signaling pathway will cause diseases. Knowledge of basic cell signaling mechanisms is therefore essential to understand pathophysiologic and pharmacologic mechanisms.

<table>
<thead>
<tr>
<th>Product Name</th>
<th>Compound Number</th>
<th>Product Features</th>
</tr>
</thead>
</table>
| HY-L037 Antioxidants Compound Library            | 800+            | • Act as antioxidants for HTS and HCS.  
• **Main targets**: NF-κB, mTOR, Keap1-Nrf2, AMPK, Sirtuin, etc.                                                                                                                                                                                                                                                                                  |
| HY-L038 Differentiation Inducing Compound Library | 1,000+          | • Act as stemness/self-renewal pathway inhibitors and differentiation activators/agonists.  
• **Main targets**: Wnt/β-catenin, Hedgehog/Gli, Jagged/Notch, BMP and retinoic acid (RA), etc.                                                                                                                                                                                                                                                   |
| HY-L039 Reprogramming Compound Library           | 1,300+          | • A unique collection of reprogramming compounds.  
• **Main targets**: Epigenetic modifiers, metabolism regulators, cell senescence alleviators and signaling pathway modulators such as Wnt, MET, Hedgehog pathways.                                                                                                                                                                                        |
| HY-L050 Ubiquitination Compound Library          | 200+            | • A unique collection of bioactive ubiquitination related compounds.  
• **Main targets**: Proteasome, E1/E2/E3 Enzyme, Deubiquitinase, p97, etc.                                                                                                                                                                                                                                                                       |
| HY-L004 Cell Cycle/DNA Damage Compound Library   | 1,200+          | • A unique collection of Cell Cycle/DNA Damage related compounds.  
• **Main targets**: CDK, ROCK, Aurora Kinase, ATM/ATR, DNA-PK, DNA/RNA Synthesis, etc.                                                                                                                                                                                                                                                              |
| HY-L005 Epigenetics Compound Library             | 800+            | • A unique collection of compounds used for epigenetics research and associated assays.  
• **Main targets**: HDAC, Histone Demethylase, HAT, DNMT, Epigenetic Reader Domain, MicroRNA, etc.                                                                                                                                                                                                                                                  |
| HY-L006 GPCR/G Protein Compound Library          | 1,600+          | • A unique collection of compounds targeting GPCRs for various research and drug development projects.  
• **Main targets**: 5-HT Receptor, Dopamine Receptor, Opioid Receptor, Adrenergic Receptors, Cannabinoid Receptor, mGluR, ETA Receptor, etc.                                                                                                                                                                      |
| HY-L024 Histone Modification Research Compound Library | 400+         | • A unique collection of bioactive compounds related to histone modification.  
• **Main targets**: Epigenetic Reader Domain, HDAC, HAT, Histone Demethylase, Histone Methyltransferase, Sirtuin, etc.                                                                                                                                                                                                                               |
<table>
<thead>
<tr>
<th>Product Name</th>
<th>Compound Number</th>
<th>Product Features</th>
</tr>
</thead>
</table>
| HY-L007 Immunology/Inflammation Compound Library       | 3,000+          | • A unique collection of bioactive compounds used for Immunology/Inflammation research.  
• **Main targets**: CCR, COX, Interleukin Related, IRAK, MyD88, PDE, PD-1/PD-L1, TLR, etc.                                                 |
| HY-L008 JAK/STAT Compound Library                      | 300+            | • A unique collection of bioactive compounds related to JAK/STAT signaling.  
• **Main targets**: JAK, STAT, EGFR, Pim, etc.                                                                                                         |
| HY-L009 Kinase Inhibitor Library                       | 2,000+          | • A unique collection of kinase inhibitors.  
• **Main targets**: Protein Kinases (VEGFR, EGFR, BTK, CDK, Akt, etc.), lipid kinases (PI3K, PI4K, SK, etc.) and Hexokinase.                                |
| HY-L010 MAPK Compound Library                          | 300+            | • A unique collection of MAPK signaling pathway inhibitors or activators.  
• **Main targets**: ERK, JNK, MEK, p38 MAPK, Raf, RSK, etc.                                                                                          |
| HY-L011 Membrane Transporter/Ion Channel Compound Library | 1,000+         | • A unique collection of compounds related to Ion Channel and Membrane Transporter research.  
• **Main targets**: Pgp, CRM1, BCRP, etc., and Ion Channels including CFTR, proton pump, sodium pump, calcium pump, etc.            |
| HY-L013 Neuronal Signaling Compound Library            | 1,700+          | • A unique collection of neuronal signaling pathways-related compounds.  
• **Main targets**: 5-HT Receptor, AChE, AMPAR, Beta-secretase, Dopamine Receptor, Melatonin Receptor, AChR, Opioid Receptor, γ-secretase, etc. |
| HY-L014 NF-κB Signaling Compound Library               | 500+            | • A unique collection of NF-κB signaling pathways-related compounds.  
• **Main targets**: IKK, Keap1-Nrf2, NF-κB, etc.                                                                                                       |
| HY-L015 PI3K/Akt/mTOR Compound Library                 | 400+            | • A unique collection of compounds used for PI3K/Akt/mTOR pathways research.  
• **Main targets**: Akt, AMPK, DNA-PK, PDK-1, mTOR, PI3K, PTEN, etc.                                                                                     |
| HY-L016 Protein Tyrosine Kinase Compound Library       | 700+            | • A unique collection of protein kinase inhibitors or activators.  
• **Main targets**: VEGFR, ALK, Btk, Bcr-Abl, c-Met/HGFR, EGFR, FGFR, Insulin Receptor, JAK, PDGFR, etc.                                                   |
<table>
<thead>
<tr>
<th>Product Name</th>
<th>Compound Number</th>
<th>Product Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>HY-L017 Stem Cell Signaling Compound Library</td>
<td>1,200+</td>
<td>• A unique collection of compounds related to stem cell regulatory and signaling pathways research.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: GSK-3, Hedgehog, Notch, JAK, ROCK, Wnt, γ-secretase, Casein Kinase, etc.</td>
</tr>
<tr>
<td>HY-L018 TGF-beta/Smad Compound Library</td>
<td>150+</td>
<td>• A unique collection of TGF-beta/Smad inhibitors or activators.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: PKC, ROCK, TGF-beta/Smad, TGF-β Receptor, etc.</td>
</tr>
<tr>
<td>HY-L045 Oxygen Sensing Compound Library</td>
<td>1,600+</td>
<td>• A unique collection of oxygen sensing related compounds.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: HIF, HIF Prolyl-Hydroxylase, E1/E2/E3 Enzyme, ROS, PI3K, MAPK, etc.</td>
</tr>
<tr>
<td>HY-L054 Endoplasmic Reticulum Stress Compound Library</td>
<td>150+</td>
<td>• A unique collection of ER stress-related compounds.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: PERK, IRE1, ATF6, etc.</td>
</tr>
<tr>
<td>HY-L020 Wnt/Hedgehog/Notch Compound Library</td>
<td>200+</td>
<td>• A unique collection of compounds used for Wnt/Hedgehog/Notch pathway research and screening.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: Notch, Gli, GSK-3, Hedgehog, Porcupine, sFRP-1, Smo, Wnt, β-catenin, etc.</td>
</tr>
<tr>
<td>HY-L060 Cytoskeleton Compound Library</td>
<td>900+</td>
<td>• A unique collection of compounds used for cytoskeleton research.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: Kinesin, Microtubule/Tubulin, Arp2/3 Complex, Bcr-Abl, etc.</td>
</tr>
<tr>
<td>HY-L062 Neurotransmitter Receptor Compound Library</td>
<td>1,200+</td>
<td>• A unique collection of compounds used for neurological diseases research.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: Neurotransmitter receptors including mAChR, nAChR, Adrenergic Receptor, Dopamine Receptor, etc.</td>
</tr>
<tr>
<td>HY-L089 Mitochondria-Targeted Compound Library</td>
<td>400+</td>
<td>• A unique collection of compounds against mitochondrial protein targets.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: Mitochondrial Metabolism, ATP Synthase, Mitophagy, Reactive Oxygen Species, etc.</td>
</tr>
<tr>
<td>Product Name</td>
<td>Compound Number</td>
<td>Product Features</td>
</tr>
<tr>
<td>------------------------------------------------</td>
<td>-----------------</td>
<td>---------------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>HY-L072 Exosomes Compound Library</td>
<td>50+</td>
<td>• A unique collection of Exosomes secretion-related compounds.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: N-SMase, PIKfyve, etc.</td>
</tr>
<tr>
<td>HY-L090 Transcription Factor Targeted Library</td>
<td>800+</td>
<td>• A unique collection of compounds with validated transcription factor targets modulating properties.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: STAT, c-Myc, Oct3/4, NF-κB, etc.</td>
</tr>
<tr>
<td>HY-L081 Phosphatase Inhibitor Library</td>
<td>100+</td>
<td>• A unique collection of phosphatase inhibitors for HTS and HCS.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: PTPs and serine/threonine-specific protein phosphatases (PP1, PP2A, and PP2B, etc.)</td>
</tr>
<tr>
<td>HY-L088 Angiogenesis Related Compound Library</td>
<td>1,300+</td>
<td>• A unique collection of compounds with validated angiogenesis targets modulating properties.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• <strong>Main targets</strong>: VEGFR, Ephrin Receptor, PDGFR, FGFR, etc.</td>
</tr>
</tbody>
</table>

Publications Citing Use of MCE Products in These Libraries

- **Cell.** 2021 Apr 15;184(8):2,167-2182.e22.
- **Cancer Res.** 2021 Apr 5;canres.3738.2020.
- **Sci Adv.** 2021 Apr 14,7(16);eabb2213.
- **Front Cell Dev Biol.** 2021 Sep 20;9:712224.
- **Elife.** 2021 Sep 29;10:e65811.
- **Cell Rep.** 2021 Jul 20;36(3):109404.
- **Small.** 2020 Jun;16(22);e2,001371.
- **Mil Med Res.** 2020 Sep 6,7(1):42.
- **Autophagy.** 2021 Jun;17(6):1426-1447.
- **Nat Protoc.** 2021 Jan;16(1):405-430.
- **Cell Prolif.** 2021 Jan;54(1):e12932.
- **Toxins.** 2021 Aug 22;13(8):585.
- **Life Sci.** 2020 Sep;1,256:117983.
- **Cell Death Differ.** 2020 Jul;27(7):2158-2175.

**Customize Library**

- Specific Compounds
- Quantities
- Plate Map
- Concentration
- Form (Solid or Solution)
Cancer is the second leading cause of death worldwide and a serious threat to human health. Dysregulation of cell cycle and cell division are the main causes of cancer. In cancer treatment, the commonly used treatment methods include chemotherapy, radiotherapy, targeted therapy, immunotherapy, surgical treatment or a combination of several treatments. Chemotherapy, as a traditional method of cancer treatment, has high side effects. In recent years, targeted therapy and tumor immunity have gradually become important means of cancer treatment. Targeted therapies play an important role in cancer treatment by targeting proteins that control the growth, division and spread of cancer cells. Tumor immunotherapy is a treatment method to eliminate tumors by activating and mobilizing the body's immune system to kill tumor cells. Immune checkpoint is a common target in tumor immunotherapy. In recent years, more and more studies have shown that tumor microenvironment plays an increasingly important role in the development of tumor, especially in the study of tumor immunity and tumor metabolism.
Cancer is the second leading cause of death globally and seriously threatens human health. A neoplasm and malignant tumor are other common names for cancer. Disruption of the normal regulation of cell-cycle progression and division lies at the heart of the events leading to cancer. Targeted therapy, which targets proteins that control how cancer cells grow, divide and spread, plays an important role in cancer treatment. Recent studies mainly focus on targeting the key proteins for cancer surviving, cancer stem cells, the tumor microenvironment and tumor immunology, etc.

Product Features

- 5,000+ compounds with anti-solid tumor and/or hematologic tumor activity, which can be used for both HTS and HCS.
- Covers diverse signaling pathways, including kinase, GPCR, epigenetics and other hot research areas.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Examples of Targets in Anti-Cancer Compound Library

- ADC Cytotoxin
- Androgen Receptor
- Autophagy
- Calcium Channel
- c-Kit
- Deubiquitinase
- EGFR
- Estrogen Receptor/ERR
- FLT3
- Histone Acetyltransferase
- IDO
- MDM-2/p53
- Mitophagy
- Notch
- Raf
- Reactive Oxygen Species
- Akt
- Antibiotic
- Bcl-2 Family
- Casein Kinase
- c-Met/HGFR
- DNA Alkylator/Crosslinker
- GSK-3
- Histone Demethylase
- HSP
- JAK
- MEK
- MMP
- Nucleoside Antimetabolite/Analog
- RET
- ALK
- Apoptosis
- Bcr-Abl
- Caspase
- COX
- DNA/RNA Synthesis
- Epigenetic Reader Domain
- Ferroptosis
- HDAC
- Histone Methyltransferase
- JNK
- Microtubule/Tubulin
- mTOR
- p38 MAPK
- ROCK
- RAR/RXR
- AMPK
- Aurora Kinase
- Btk
- CDK
- Cytochrome P450
- E1/E2/E3 Enzyme
- ERK
- FGFR
- HIF/HIF Prolyl-Hydroxylase
- Keap1-Nrf2
- Mitochondrial Metabolism
- NF-κB
- PARP
- Ras
- Sirtuin
- Src
Immuno-Oncology is a type of immunotherapy that has the specific way of treating cancer. It works by stimulating our immune system to fight back. Normally, our immune system is able to destroy cancer cells in our body, however sometimes cancer cells can adapt and mutate, effectively hiding from our immune system. This is when tumors can develop and become a threat to our health. Immuno-oncology involves mobilizing lymphocytes to recognize and eliminate cancer cells using the body’s immune system. There are several immuno-oncology treatments available, including Immune cell therapy (CAR-T), monoclonal antibodies (mABs) and checkpoint inhibitors, cytokines and cancer vaccines.

**Product Features**

- **300+** bioactive tumor immunology compounds that target some important checkpoints such as PD1/PD-L1, CXCR, Sting, IDO, TLR, etc.
- A useful tool for cancer research by activation of antitumor immune response.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- Detailed compound information with structure, target and brief introduction.
- High purity and quality validated by NMR and LC/MS.

**Examples of Targets in Small Molecule Immuno-Oncology Compound Library**

- PD-1/PD-L1
- STING
- IDO
- CXCR
- Wnt
- TGF-β
- PTEN
- Hedgehog
- TLR
- CTLA4
Breast cancer is the most frequent cancer among women, impacting 2.1 million women each year, and also causes the greatest number of cancer-related deaths among women. Breast cancer is a heterogeneous disease, which is categorized into 3 major subtypes based on the presence or absence of molecular markers for estrogen or progesterone receptors and human epidermal growth factor 2 (ERBB2; formerly HER2): hormone receptor positive/ERBB2 negative (70% of patients), ERBB2 positive (15%-20%), and triple-negative (tumors lacking all 3 standard molecular markers; 15%).

HER2, Estrogen Receptor, CDK, VEGFR, PI3K are commonly used targets in breast cancer treatment and are also important targets in anti-breast cancer drug discovery.

Product Features

- According to the analysis of the clinical and approved drugs used in breast cancer treatment, the targets commonly used in the treatment of breast cancer are collected. Based on these targets, MCE carefully collects 1,300+ compounds that have potential anti-breast cancer activity.
- Mainly target EGFR, VEGFR, Estrogen Receptor, PI3K, AKT, JAK, STAT, PD-1/PD-L1, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- Detailed compound information with structure, target and brief introduction.
- High purity and quality validated by NMR and LC/MS.

Some examples of targets in MCE Anti-Breast Cancer Compound Library
Lung cancer is a major global health problem, as it is the leading cause of cancer-related deaths worldwide. Lung cancer may be treated with surgery, chemotherapy, radiation therapy, targeted therapy, immunotherapy or a combination thereof. Targeted therapy is one of the most exciting developments in lung cancer medicine, especially for NSCLC. Extensive genomic characterization of NSCLC has led to the identification of molecular subtypes of NSCLC that are oncogene addicted and exquisitely sensitive to targeted therapies. These include activating mutations in epidermal growth factor receptor (EGFR) and BRAF or echinoderm microtubule-associated protein-like 4 (EML4)-anaplastic lymphoma kinase (ALK) fusions and ROS1 receptor tyrosine kinase fusions. These are important targets for targeted therapy.

### Product Features

- According to the analysis of the clinical and approved drugs used in lung cancer treatment, the targets commonly used in the treatment of lung cancer are collected. Based on these targets, we carefully collect 1,200+ compounds that have potential anti-lung cancer activity.
- Mainly target EGFR, VEGFR, Estrogen Receptor, PI3K, AKT, JAK, STAT, PD-1/PD-L1, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

<table>
<thead>
<tr>
<th>Target</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PI3K</td>
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</tr>
<tr>
<td>EGFR</td>
<td>20</td>
</tr>
<tr>
<td>mTOR</td>
<td>40</td>
</tr>
<tr>
<td>AKT</td>
<td>60</td>
</tr>
<tr>
<td>FGFR</td>
<td>80</td>
</tr>
<tr>
<td>VEGFR</td>
<td>100</td>
</tr>
<tr>
<td>c-Met/HGFR</td>
<td>120</td>
</tr>
<tr>
<td>BRAF</td>
<td>140</td>
</tr>
<tr>
<td>PDGFR</td>
<td>80</td>
</tr>
<tr>
<td>ALK</td>
<td>100</td>
</tr>
<tr>
<td>KRAS</td>
<td>120</td>
</tr>
<tr>
<td>RET</td>
<td>140</td>
</tr>
<tr>
<td>c-Kit</td>
<td>80</td>
</tr>
<tr>
<td>ROS</td>
<td>100</td>
</tr>
</tbody>
</table>

Some examples of targets in MCE Anti-Lung Cancer Compound Library
Pancreatic cancer is a devastating disease with a low overall survival rate. Chemotherapy is the most common treatment for patients presenting with advanced pancreatic cancer. More recently, the era of targeted therapies has generated a lot of interest in discovering better approaches for patients with pancreatic cancer. Commonly mutated genes in pancreatic cancer include K-ras (in 74-100% of cases), p16INK4a (up to 98%), p53 (43 to 76%), DPC4 (about 50%), HER-2/neu (in about 65%) and FHIT (found in 70% of cases). Other genes include notch1, Akt-2, BRCA2 and COX-2. These proteins are important targets of target therapies for pancreatic cancer.

Product Features

- According to the analysis of the clinical and approved drugs used in pancreatic cancer treatment, the targets commonly used in the treatment of pancreatic cancer are collected. Based on these targets, MCE carefully collects 1,600+ compounds that have potential anti-pancreatic cancer activity.
- Mainly target EGFR, ALK, ROS1, c-MET/HGFR, RET, FGFR, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.
Some examples of targets in MCE

**Anti-Blood Cancer Compound Library**

(96-/384-well plate)

Blood cancers, also called hematologic cancers, occur when abnormal blood cells start growing out of control, interrupting the function of normal blood cells, which fight off infection and produce new blood cells. Most blood cancers start in the bone marrow, which is where blood is produced. There are three main types of blood cancers: leukemia, lymphoma and myeloma, which afflict millions of children and adults every year, and are often deadly.

**Product Features**

- According to the analysis of the clinical and approved drugs used in blood cancer treatment, the targets commonly used in the treatment of blood cancer are collected. Based on these targets, MCE carefully collects **1,800+** compounds that have potential anti-blood cancer activity.
- Mainly target EGFR, ALK, ROS1, c-MET /HGFR, RET, FGFR, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- Detailed compound information with structure, target and brief introduction.
- High purity and quality validated by NMR and LC/MS.

<table>
<thead>
<tr>
<th>Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>CDK</td>
</tr>
<tr>
<td>PI3K</td>
</tr>
<tr>
<td>Epigenetic Reader Domain</td>
</tr>
<tr>
<td>VEGFR</td>
</tr>
<tr>
<td>Histone Methyltransferase</td>
</tr>
<tr>
<td>HDAC</td>
</tr>
<tr>
<td>JAK</td>
</tr>
<tr>
<td>Nucleoside Antimetabolite/Analog</td>
</tr>
<tr>
<td>mTOR</td>
</tr>
<tr>
<td>AKT</td>
</tr>
<tr>
<td>STAT</td>
</tr>
<tr>
<td>FLT3</td>
</tr>
<tr>
<td>Bcl-2 Family</td>
</tr>
<tr>
<td>c-Kit</td>
</tr>
</tbody>
</table>

**Publications Citing Use of MCE Products in This Library**

- *Cancer Sci.* 2021 Mar;112(3):997-1010
- *J Immunother Cancer.* 2021 Jul;9(7):e001758
- *Theranostics.* 2021 Mar 24;11(12):5650-5674
The paramount hallmark of tumor metabolism is "aerobic glycolysis" or the Warburg effect, coined by Otto Warburg in 1926, in which cancer cells produce most of their energy from the glycolysis pathway regardless of whether in aerobic or anaerobic conditions. Usually, cancer cells are highly glycolytic and take up more glucose than do normal cells from outside. The increased uptake is facilitated by the overexpression of several isoforms of membrane glucose transporters (GLUTs). Likewise, the metabolic pathways of glutamine, amino acid and fat metabolism are also altered. Recent trends suggest that targeting the altered metabolic pathways of cancer cells results in an energy crisis inside the cancer cells and can selectively inhibit cancer cell proliferation by delaying or suppressing tumor growth.

Targeted cancer therapies are drugs or other substances that block the growth and spread of cancer by interfering with specific molecular targets that are involved in the growth, progression, and spread of cancer. There are several different types of targeted therapy. The most common types are small-molecule drugs and monoclonal antibodies. Because of high specificity, low side effects, and potent anticancer activity, targeted therapy has become the mainstream of new anti-tumor drugs. Various targeted therapies have been approved by FDA and used in the treatment of diseases.

Product Features

- A unique collection of 100+ approved targeted therapeutic small molecule drugs which can be used for HTS and HCS.
- Mainly target EGFR, Bcr-Abl, ALK, JAK, Epigenetics, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Anti-Cancer Metabolic Compounds Library

(96-/384-well plate)

The paramount hallmark of tumor metabolism is "aerobic glycolysis" or the Warburg effect, coined by Otto Warburg in 1926, in which cancer cells produce most of their energy from the glycolysis pathway regardless of whether in aerobic or anaerobic conditions. Usually, cancer cells are highly glycolytic and take up more glucose than do normal cells from outside. The increased uptake is facilitated by the overexpression of several isoforms of membrane glucose transporters (GLUTs). Likewise, the metabolic pathways of glutamine, amino acid and fat metabolism are also altered. Recent trends suggest that targeting the altered metabolic pathways of cancer cells results in an energy crisis inside the cancer cells and can selectively inhibit cancer cell proliferation by delaying or suppressing tumor growth.

Product Features

- A unique collection of 800+ tumor metabolism-related small molecule compounds, which can be used for anti-cancer metabolism targets identification, validation as well as anti-cancer drug discovery.
- Covers various signaling pathways and targets related to tumor metabolism, such as glucose metabolism, glutamine metabolism, amino acid metabolism, fat metabolism, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.
Anti-Infection Series

An infection occurs when another organism enters a person's body and causes disease. The organisms that cause infections are very diverse and can include things like viruses, bacteria, fungi, and parasites. The immune system is an effective barrier against infectious agents.

MCE provides a unique collection of anti-infective compounds with detailed classification by anti-bacterial, anti-viral, anti-fungal and anti-parasite activities. You can choose based on your need:

- HY-L002 Anti-Infection Compound Library
- HY-L027 Antiviral Compound Library
- HY-L049 Antibacterial Compound Library
- HY-L067 Antibiotics Library
- HY-L048 Antifungal Compound Library
- HY-L082 Antiparasitic Compound Library
- HY-L073 Anti-Hepatitis C Virus Compound Library
- HY-L052 Anti-COVID-19 Compound Library

An infection occurs when another organism enters a person’s body and causes disease. The organisms that cause infections are very diverse and can include things like viruses, bacteria, fungi, and parasites. The immune system is an effective barrier against infectious agents.

**Product Features**

- **1,800+** bioactive anti-infection (anti-bacteria, anti-fungi, anti-parasite and anti-virus) compounds that could be used for HTS and HCS.
- Structurally diverse, medicinally active, and cell-permeable.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- Detailed bioactivity information, including target, research areas, clinical information.
- High purity and quality validated by NMR and LC/MS.

**Product Features**

- A unique collection of **600+** bioactive anti-virus compounds for HTS and HCS.
- Mainly target HBV, HCV, HIV, HSV, Influenza Virus, Reverse Transcriptase, etc.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- Detailed bioactivity information, including target, research areas, clinical information.
- High purity and quality validated by NMR and LC/MS.
Antibacterial agents are a group of materials that fight against pathogenic bacteria. Thus, by killing or reducing the metabolic activity of bacteria, their pathogenic effect in the biological environments will be minimized. The most widely used antibacterial agents exert their effects on bacterial cell wall synthesis, protein synthesis, DNA replication, and metabolic pathways. However, resistance to antimicrobial agents has become a major source of morbidity and mortality worldwide. The main mechanisms of resistance are limiting uptake of a drug, modification of a drug target, inactivation of a drug, and active efflux of a drug. Therefore, it is an urgent need to develop new drugs targeted at resistant organisms.

**Product Features**

- **800+** compounds have definite antibacterial activity and can be used for HTS and HCS.
- Act on various targets of bacteria, such as *cell wall*, *cell membranes*, *ribosomes*, *nucleic acids*, *bacterial cellular metabolism*, and *bacterial cellular enzymes*.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

**Examples of Compounds with Different Mechanisms of Action**

- **Inhibition of Cell wall synthesis**
  - D-Cycloserine (HY-B0030)
  - Cefazolin (HY-B1596)
  - Cefpodoxime Proxetil (HY-N7101)
  - Meropenem (HY-13678A)

- **Inhibition of Cell-membrane function**
  - Chlorhexidine (HY-B1248)
  - Colistin (HY-A0089)
  - SPR206 (HY-128780B)

- **Inhibition of bacterial cellular metabolism**
  - Trimethoprim (HY-B0510)
  - Pralatrexate (HY-10446)
  - Diaveridine (HY-B1902)
  - Proguanil (HY-B0806)

- **Inhibition of DNA synthesis**
  - Nalidixic acid (HY-B0398)
  - Enoxacin (HY-B0268A)
  - Pefloxacin (HY-B0147A)
  - Trovafloxacin (HY-A0170)

- **Inhibition of RNA synthesis**
  - Mupirocin (HY-B0958)
  - Rifabutin (HY-17025)
  - Rifalazil (HY-105099)

- **Inhibition of Protein synthesis (50S)**
  - Erythromycin (HY-B0220)
  - Pleurotomulin (HY-N2301)
  - Valnemulin (HY-B0027)
  - Ribostamycin (HY-B1228)

- **Inhibition of Protein synthesis (30S)**
  - Minocycline (HY-B0958)
  - Neomycin (HY-B0470)
  - Spectinomycin (HY-B0438)

Classes of antibiotics/antibacterial agents and their modes of action on bacteria
Antibiotics Library
(96-/384-well plate)

Product Features

- **500+ antibiotics** that can be used for HTS and HCS.
- Structurally diverse, including penicillins, cephalosporins, tetracyclines, macrolides, etc.
- Act on various targets on bacteria, such as **cell wall, cell membranes, ribosomes, nucleic acids, bacterial cellular metabolism** and **bacterial cellular enzymes**.
- Can be used in the study of new indications and the development of new anti-bacteria and anti-tumor drugs.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Examples of Antibiotics

<table>
<thead>
<tr>
<th>Cephalosporins</th>
<th>Aminoglycosides</th>
<th>Penicillins</th>
</tr>
</thead>
<tbody>
<tr>
<td>HY-108402</td>
<td>HY-16566A</td>
<td>HY-B0467A</td>
</tr>
<tr>
<td>Cefodizime</td>
<td>Kanamycin sulfate</td>
<td>Amoxicillin</td>
</tr>
<tr>
<td>HY-128932</td>
<td>HY-B0441</td>
<td>Ampicillin</td>
</tr>
<tr>
<td>Cefminox sodium</td>
<td>Tobramycin</td>
<td>Penicillin G Procaine</td>
</tr>
<tr>
<td>HY-B0200</td>
<td>HY-B1174</td>
<td></td>
</tr>
</tbody>
</table>
Examples of Antifungal Agents and Their Modes of Action on Fungi

- Inhibition of Cell wall synthesis
  - Enfumafungin (HY-N8537)
  - (S,S)-Valifenalate (HY-17518A)
  - Dimethomorph (HY-0846)

- Inhibition of mitochondrial function
  - Nerol (HY-N7063)
  - Devimista (HY-15453)

- Inhibition of Hsp90 activity
  - Tanespimycin (HY-10211)
  - Geldanamycin (HY-15230)
  - Ganetespib (HY-15205)

- Increase ROS production
  - Diallyl Trisulfide (HY-117235)
  - Camalexin (HY-119502)
  - Hexaconazole (HY-A0278)

- Inhibition of Microtubule Syntheses
  - Epothilone B (HY-17029)
  - Epothilone D (HY-15278)
  - Cytochalasin A (HY-N6773)

- Inhibition of Protein synthesis
  - Reveromycin (HY-129337)
  - Sordarin sodium (HY-126396)
  - AN2718 (HY-100527)

- Inhibition of DNA synthesis
  - Quinizarin (HY-D0226)
  - Pentamidine (HY-B05378)
  - Chromomycin A3 (HY-W040129)
  - Tunicamycin (HY-A0098)

- Inhibition of Ergosterol synthesis
  - Fenticonazole Nitrate (HY-B0359)
  - Isavuconazole (HY-14273)
  - Itraconazole (HY-17514)
  - Propiconazole (HY-B0847)

- Inhibition of DNA synthesis
  - Tacrolimus (HY-13756)
  - Fenvaletarate (HY-B0206)
  - Cyclosporin A (HY-B0579)

Old and new targets as antifungal candidates
Product Features

- **300+** compounds that can be used for HTS and HCS.
- Compounds in this library have a variety of antiparasitic activities, including **anti-plasmodium**, **anti-leishmania**, **anti-filaria**, and **anti-lymphatic filariasis**, etc.
- The compound library can be used for the study of new indications and the development of new antiparasitic drugs.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L082

**Antiparasitic Compound Library**

(96-/384-well plate)

A parasite is an organism that lives on or in a host organism and gets its food from or at the expense of its host. Parasites of humans include protozoans, helminths, and ectoparasites. They are responsible for many diseases and are transmitted to their hosts most often through the ingestion of contaminated food, water or through the bite of an arthropod (e.g., a fly or tick), which can act as an intermediate host and as a vector. Parasitic diseases of humans are a major global health problem, especially in developing countries. Each year there are hundreds of millions of people infected with disease-causing parasites, particularly in tropical and subtropical regions of the world, resulting in an estimated one million deaths.

Product Features

- **300+** compounds that can be used for HTS and HCS.
- Compounds in this library have a variety of antiparasitic activities, including **anti-plasmodium**, **anti-leishmania**, **anti-filaria**, and **anti-lymphatic filariasis**, etc.
- The compound library can be used for the study of new indications and the development of new antiparasitic drugs.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L073

**Anti-Hepatitis C Virus Compound Library**

(96-/384-well plate)

Globally, an estimated 71 million people have chronic hepatitis C virus infection. A significant number of those who are chronically infected will develop cirrhosis or liver cancer. To date, there is no vaccine against HCV. More recently, new therapeutic approaches that target essential components of the HCV life cycle have been developed, including direct-acting antiviral (DAA) that specifically block a viral enzyme or functional protein and host-targeted agents (HTA) that block interactions between host proteins and viral components that are essential to the viral life cycle. However, the genetic diversity of HCV viruses and the stage of liver disease (i.e., cirrhosis) are revealing themselves as obstacles for effective, pan-genotypic treatments. There still exists a need for the discovery and development of new HCV inhibitors.

Product Features:

- **200+** bioactive anti-hepatitis C virus compounds that can be used for HTS and HCS.
- Act on the main targets in HCV treatment, including **NS3, NS4A, NS5A**, RNA-dependent **RNA-polymerases**, **EGFR**, etc.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.
COVID-19 poses a serious threat to people’s health, and it is urgent to develop drugs to treat COVID-19 effectively. The screening of anti-COVID-19 drugs by using the clinical and approved compounds can greatly shorten the research and development cycle. Taking advantage of our virtual screening, MCE conducted virtual screening of approved compound library and clinical compound library based on the 3CL protease (PDB ID: 6LU7), Spike Glycoprotein (PDB ID: 6VSB), NSP15 (PDB ID: 6VWW), RDRP, PLPro and ACE2 structure. MCE designed a unique collection of compounds which may have anti-COVID-19 activity. The Library will be a powerful tool for screening new anti-COVID-19 drugs.

**Product Features**

- 1,500+ compounds are derived from virtual screening of approved compound library and clinical compound library based on the 3CL protease, Spike Glycoprotein and ACE2 structure.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research.

**FAQ**

— Do all the products in this library have definite anti-COVID-19 activity?

Compounds in this library were obtained by virtual screening based on the main targets of COVID-19. These compounds have potential anti-COVID-19 activity. However, there is no guarantee that all the products have anti-COVID-19 activity.

— Have these products entered the clinical trial in the anti-COVID-19 study?

The products in the library are in clinical trials or approved in other disease studies, but are not used in COVID-19 study. These products can be used to develop new indications for COVID-19 and speed up the development of anti-COVID-19 drugs based on the data and safety validation of these products in other diseases.
Neurodegenerative Disease Series

Neurodegenerative diseases are characterized by progressive dysfunction and death of neurons and include a broad range of conditions, from Parkinson’s (PD), Alzheimer’s (AD), Huntington’s disease (HD) to glaucoma. AD and PD mainly occur in middle-age and old people while HD, amyotrophic lateral sclerosis and spinal muscular atrophy may occur at any ages. At present, the cause of such diseases is not clear and there is no cure, and it is a serious threat to human health.

Recent research findings have led to a greater understanding of neurodegenerative diseases. Current studies on the pathogenesis of neurodegenerative diseases mainly include protein misfolding and aggregation, neuroinflammation, programmed cell death and aging, etc. These results not only provide useful information for elucidating the mechanism of these diseases, but also provide new ideas and targets for finding new drugs.

Major Neurodegenerative diseases, their associated regions, and current therapeutic interventions. [1]

- **Alzheimer’s disease**
  - Cortex
  - Hippocampus
  - Gotepizil
  - Rivastigmine

- **Parkinson’s disease**
  - Substantia Nigra
  - Cortex
  - Levodopa+Carbidopa
  - Pergolide
  - Bromocriptine

- **Huntington’s disease**
  - Striatum
  - Basal Ganglia
  - Reserpine
  - Phenothiazines

- **Multiple sclerosis**
  - Basal Ganglia
  - Brain Stem
  - Tysabri
  - Interferones
  - Glatiramer Acetate

Neuroprotection is an approach to prevent neurons from different pathological damages in neurodegenerative diseases.

Main targets: Calcium channel, sodium channel, adenosine A1 receptor, PI3K, etc.

Several important mechanisms have been proposed to explain the underlying pathology of AD, such as Amyloid cascade hypothesis, Tau hypothesis and Cholinergic hypothesis, etc.

MCE carefully collects 900+ compounds that have potential anti-Alzheimer’s disease activity.

Main targets: Amyloid-β, 5-HT Receptor, nAChR, etc.

Compounds with anti-Parkinson’s Disease activities or targeting the unique targets of PD which is a useful tool for exploring the mechanism of PD and discovering new drugs for PD.

Main targets: Dopamine Receptor, LRRK2, 5-HT Receptor, Monoamine Oxidase, nAChR, etc.

Compounds with anti-Neurodegenerative Diseases activities or targeting the unique targets of neurodegenerative diseases.

Main targets: Dopamine receptor, Amyloid β, COMT, LRRK2, nAChR, 5-HT receptor, Monoamine Oxidase, Histamine Receptor, etc.
# Other Disease Related Compound Libraries
(96-/384-well plate)

<table>
<thead>
<tr>
<th>Product Name</th>
<th>Compound Number</th>
<th>Product Features</th>
</tr>
</thead>
</table>
| **HY-L034 Anti-Aging Compound Library** | 2,700+          | - Bioactive anti-aging compounds.  
- **Main targets**: Sirtuin, mTOR, IGF-1R, AMPK, p53, Telomerase, Mitophagy, Mitochondrial Metabolism, COX, Cytochrome P450, Oxidase, etc. |
| **HY-L046 Anti-Cardiovascular Disease Compound Library** | 900+            | - Bioactive anti-cardiovascular compounds for HTS and HCS.  
- **Main targets**: Metabolic enzyme, membrane transporter, ion channel, inflammation related signaling pathways, etc. |
| **HY-L047 Endocrinology Compound Library** | 750+            | - Bioactive compounds which can be used in the research of endocrine regulation.  
- **Main targets**: Thyroid hormone receptor, TSH receptor, GNRH receptor and adrenergic receptor related signaling pathways. |
| **HY-L040 Diabetes Related Compound Library** | 500+            | - Diabetes-related compounds.  
- **Main targets**: SGLT, PPAR, DPP-4, AMPK, Dipeptidyl Peptidase, Glucagon Receptor, etc. |
| **HY-L087 Anti-Obesity Compound Library** | 400+            | - Compounds that mainly target signaling pathway of controlling appetite, fatty acid metabolism and energy expenditure, etc.  
- **Main targets**: Fatty Acid Synthase (FASN), GLP-1R, Adrenergic receptor, MCHR1 (GPR24), Neuropeptide Y receptor, PARP, etc. |
## Virtual Screening Database

<table>
<thead>
<tr>
<th>Library Name</th>
<th>Compound Quantity</th>
<th>Product Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCE Bioactive Compound Library</td>
<td>14,000+</td>
<td>A unique collection of 14000+ bioactive and structurally diverse compounds. Bioactivity and safety confirmed by preclinical research and clinical trials. Some have been approved by FDA.</td>
</tr>
<tr>
<td>MCE Fragment Library</td>
<td>16,000+</td>
<td>Latest release of Ro3 Fragment Library comprising over 16,000+ high-quality molecules. A useful tool for the fragment-based approach to drug discovery (FBDD).</td>
</tr>
<tr>
<td>Chemspace Lead-Like Compound Library</td>
<td>981,244</td>
<td>Chemspace Lead-Like Compound Library contains 981,244 in-Stock lead-like compounds with favorable physicochemical profiles and high Quantitative Estimation of Drug-likeness.</td>
</tr>
<tr>
<td>Chemspace Scaffold derived set</td>
<td>10,119</td>
<td>Composed of 10,119 compounds, which including 3,373 scaffolds, 3 compounds per each.</td>
</tr>
<tr>
<td>Chinese National Compound Library</td>
<td>1,398,968</td>
<td>~1.4 million compounds possessing diversified structures.</td>
</tr>
<tr>
<td>FCH Group Screening Library</td>
<td>2,244,487</td>
<td>FCH Group Screening Library contains about 2,244,487 lead-like compounds for biological screening.</td>
</tr>
<tr>
<td>InterBioScreen Synthetic Compounds Library</td>
<td>485,000</td>
<td>InterBioScreen Synthetic Compounds Library contains about 485,000 immediately available compounds.</td>
</tr>
<tr>
<td>Life Chemicals HTS Compound Collection</td>
<td>494,471</td>
<td>Life Chemicals HTS library is a unique collection contains 494,471 diverse screening compounds for the lead identification via high-throughput screening (HTS) and high content screening (HCS).</td>
</tr>
<tr>
<td>OTAVAchemicals Screening Collection</td>
<td>270,000</td>
<td>OTAVAchemicals Screening Collection contains about 270,000 re-supply compounds for prompt delivery.</td>
</tr>
</tbody>
</table>
## Virtual Screening Database

<table>
<thead>
<tr>
<th>Library Name</th>
<th>Compound Quantity</th>
<th>Product Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specs HTS Compounds Library</td>
<td>208,518</td>
<td>Specs HTS library is a unique collection contains 208,518 diverse screening compounds for the lead identification via high-throughput screening (HTS) and high content screening (HCS).</td>
</tr>
<tr>
<td>UORSY New Generation Screening Library</td>
<td>1,900,000</td>
<td>UORSY New Generation Screening Library contains about 1,900,000 compounds. The library is a revolutionary collection of lead-like molecules with outstanding structural quality and diversity—New Generation Screening Library (NGSL).</td>
</tr>
<tr>
<td>UORSY Screening Library</td>
<td>680,000</td>
<td>UORSY Screening Library contains about 680,000 compounds. The library has extensively developed a polymerization synthesis method that provides a highly diverse chemical structure.</td>
</tr>
<tr>
<td>Vitas-M Screening Compounds Library</td>
<td>1,400,000</td>
<td>Stock of synthetic small molecule organic compounds for biological screening and lead optimization. It is the best source to make “cherry pick” selection as per your criteria.</td>
</tr>
</tbody>
</table>

### Customize Library

**You can select**
- Specific Compounds
- Quantities
- Plate Map
- Concentration
- Form (Solid or Solution)